UCRL-JC-126022 Abs

Abstract submitted for
1997 APS March Meeting,
17-21, March 1997, Kansas City, MO

Sorting catagory - 16 g

Symmetric Hydrogen Bonds in Hydrous Magnesium Silicate at High Pressures*

Hyunchae Cynn and Choong-Shik Yoo
Lawrence Livermore National Laboratory
Ann Hofmeister
Washington University

The stability of water contained in silicates is crucial for understanding the planetary evolution. The nature of hydrogen bonding in hydrous magnesium silicate (often called as "phase B") has been studied to 40 GPa by using vibrational spectroscopy. In this paper, we present the first experimental result showing that hydrogen bonds in phase B symmetrize at high pressures between 6 and 30 GPa. Two major OH vibration bands at 3411 and 3352 cm-1 initially soften with increasing pressure, which in turn harden above 7 and 30 GPa, respectively. Such a turnover in the OH stretching modes suggests that hydrogen atom occupies the mid-point of two adjacent oxygen atoms. The crystallographic data indicate that the symmetrization occurs at the critical OH-bond distance of 2.8 Å. In contrast to the phase transition in ice VII, there is no indication of the1st order phase transition associated with the OH symmetrization in phase B.

* Part of this work performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.